Pair contact process with diffusion of pairs

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Abstract

The pair contact process (PCP) is a nonequilibrium stochastic model which, like the basic contact process (CP), exhibits a phase transition to an absorbing state. The two models belong to the directed percolation (DP) universality class, despite the fact that the PCP possesses infinitely many absorbing configurations whereas the CP has but one. The critical behavior of the PCP with hopping by particles (PCPD) is as yet unclear. Here we study a version of the PCP in which nearest-neighbor particle *pairs* can hop but individual particles cannot. Using quasistationary simulations for three values of the diffusion probability ($D = 0.1$, 0.5 and 0.9), we find convincing evidence of DP-like critical behavior.

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I. INTRODUCTION

The exploration of universality classes associated with nonequilibrium phase transitions continues to attract much interest [1–3]. In the case of systems exhibiting a phase transitions to an absorbing state, the generic universality class is that of directed percolation (DP) [4, 5]. For example, both the basic contact process (CP) [6] and the pair contact process (PCP) [7, 8] belong to this class, despite the fact that the former has a unique absorbing configuration while the latter possesses infinitely many. Allowing individual particles to hop in the PCP, one obtains the so-called pair contact process with diffusion (PCPD). In this case there are only two absorbing states: the empty lattice, and the state of a single particle hopping.

A model with the basic features of the PCPD was first proposed by Grassberger in 1982. More recent interest in this problem was stimulated by the work of Howard and Täuber [9] who discussed a generalized version, with a Langevin description involving complex noise. On the basis of numerical results, Carlon *et al.* [10], suggested that the critical behavior of the PCPD would fall in the parity-conserving (PC) class. Subsequent works [11, 12] suggested a different kind of critical behavior, possibly masked by huge corrections to scaling. (For a comprehensive review of analyses of the PCPD up to 2004, see the article by Henkel and Hinrichsen [13].)

Given the controversies surrounding the PCPD, it seems worth checking whether allowing hopping by pairs (*only*) changes the critical behavior of the PCP. One expects such a model to remain in the DP universality class, given that the critical behavior of the CP is robust to the inclusion of nearest-neighbor hopping [14]. Note as well that pairwise diffusion does not change the set of absorbing configurations in the PCP. In the present work, we study a variant of the PCP in which nearest neighbor pairs of particles may hop together, while isolated particles cannot hop. Using quasistationary (QS) simulations, we determine several critical parameters for three values of the diffusion probability: $D = 0.1, 0.5$ and 0.9. The balance of this paper is organized as follows. In Sec. II we define the model and detail our simulation method. In Sec. III we present our results; Sec. IV is devoted to discussion and conclusions.

II. MODEL AND SIMULATION METHOD

The CP [1, 6] is one of the simplest and most studied models belonging to the DP universality class. In the CP, each site i of a lattice is either occupied [$\sigma_i(t) = 1$] or vacant [$\sigma_i(t) = 0$]. Transitions from $\sigma_i = 1$ to 0 occur at a rate of unity, independent of the neighboring sites. The reverse transition can only occur if at least one neighbor is occupied: the transition from $\sigma_i = 0$ to 1 occurs at rate λm, where m is the fraction of nearest neighbors of site i that are occupied; thus the state $\sigma_i = 0$ for all i is absorbing. λ is the only control parameter in the basic CP; the order parameter ρ is the fraction of occupied sites.

The PCP [7, 8] is defined on a d-dimensional lattice, with each site again either occupied or vacant. Only pairs of particles occupying nearest-neighbor sites exhibit activity: each such pair has a rate $1 - p$ of mutual annihilation, and a rate p to create a new particle at a randomly chosen site neighboring the pair, if this site is vacant. In the PCPD [10], in addition to the creation and annihilation processes present in the PCP, each particle attempts to hop, at rate D, to a randomly chosen nearest-neighbor (NN) site; the move is accepted if the target site is vacant. Several variants of the model, differing in how each process (creation, annihilation or diffusion) is selected, have been studied [13].

The model studied here, pair contact process with diffusion of pairs (PCPDP), again features the pair-mediated annihilation and creation processes of the PCP. In addition, a fraction D of all events are hopping attempts by a NN particle pair. The model is defined on a ring of L sites. The transition rates associated with each pair (AA) are:

$$\begin{aligned} &\emptyset AA \to AA\emptyset, \quad AA\emptyset \to \emptyset AA, && \text{at rate } D/2 \\ &AA\emptyset, \ \ \emptyset AA \to AAA, && \text{at rate } p(1-D)/2 \\ &AA \to \emptyset\emptyset, && \text{at rate } (1-p)(1-D). \end{aligned} \tag{1}$$

Thus hopping ceases, along with all other activity, in the absence of pairs.

The most obvious definition of the order parameter in the PCPDP is the pair density ρ_p, that is, the number of nearest-neighbor occupied pairs divided by the total number of nearest-neighbor pairs on the lattice (on the ring, the latter is equal to the number of sites). Since the number of particles can only change in the presence of pairs, one might expect the

excess particle density, $\Delta\rho_{part} = \rho_{part} - \rho_{part,c}$, to scale in a similar manner. (Note that the critical particle density $\rho_{part,c}$ is nonzero [7].) We confirm that $\Delta\rho_{part}$ and ρ_p exhibit similar scaling properties.

We sample the quasistationary (QS) distribution of the process, i.e., conditioned on survival, using a simulation method that yields quasistationary properties directly [15]. This is done by maintaining, and gradually updating, a set of configurations visited during the evolution; when a transition to the absorbing state is imminent the systems is instead placed in one of the saved configurations. Otherwise the evolution is identical to that of a conventional simulation. The set of saved configurations is updated by replacing with a small probability, p_{rep}, at each time step, one of the saved configurations with the current one.

We perform extensive simulations of the one-dimensional PCPDP, using systems of $L = 10, 20, 40, 80, 160, 320, 640$ sites, using the QS simulation method. Each realization of the process is initialized with all sites occupied, and runs for 5×10^6 to 10^8 time steps (longer runs for larger systems). Our results are calculated over samples sizes 10-20 realizations. The number of saved configurations ranges from 100 to 1000 (larger numbers for smaller systems). Values of p_{rep} range from 10^{-3} to 5×10^{-4} (smaller values for larger systems). During the relaxation phase we use a p_{rep} ten times larger, to eliminate the influence of the initial configuration. Following this relaxation phase, we accumulate histograms of the time during which the system has exactly $1, 2, ..., n, ...$ pairs, and similarly for particles. Using the histograms we calculate the densities of pairs and of particles, the moment ratio $m \equiv \langle\rho_p^2\rangle/\langle\rho_p\rangle^2$ and the reduced fourth cumulant $q_4 \equiv K_4/K_2^2$, where $K_2 = \mathrm{var}(\rho_p)$ and,

$$K_4 = \langle\rho_p^4\rangle - 4\langle\rho_p^3\rangle\langle\rho_p\rangle - 3\langle\rho_p^2\rangle^2 + 12\langle\rho_p^2\rangle\langle\rho_p\rangle^2 - 6\langle\rho_p\rangle^4. \tag{2}$$

The QS lifetime τ is taken as the mean time between attempts to visit an absorbing configuration.

III. SIMULATION RESULTS

For each diffusion rate studied, the first step in the analysis is to determine the critical annihilation probability $p_c(D)$. Experience with absorbing-state phase transitions leads us to expect the following scaling properties at the critical point: $\rho_p \sim L^{-\beta/\nu_\perp}$; $\tau \sim L^z$; and

$m(L) \to m_c$, a universal critical value [16]. We obtain a preliminary estimate of p_c from the crossing of the moment ratios m for system sizes $L = 10$ and 20, and then concentrate our efforts in simulations near this value. (For $D = 0.5$, for example, we focus on the interval $p \in [0.85, 0.90]$, see Fig. 1).

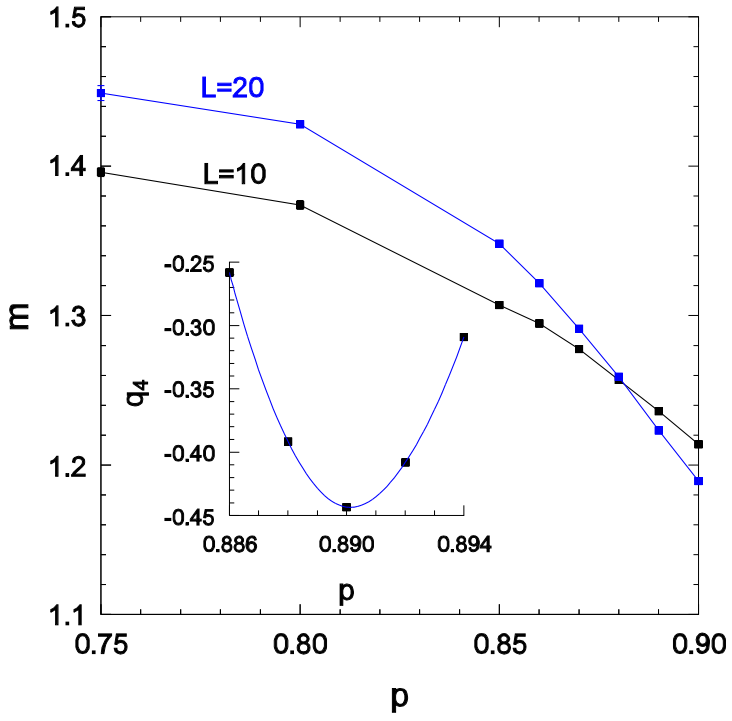

FIG. 1: (Color online) Moment ratio m versus creation parameter p for $D = 0.5$, $L = 10$, 20. Inset: Reduced fourth cumulant versus p for $L = 160$, $D = 0.5$.

For each pair of consecutive lattice sizes, L and $2L$, we determine the crossing values $p_\times$ and $m_\times$. An independent estimate of the critical point is afforded by the reduced fourth cumulant, q_4, which takes a pronounced minimum at a value $p_q(L)$ that converges to the critical value; see Fig. 1, inset. In Fig. 2 we plot $p_\times$ and p_q versus $1/L$, for $D = 0.5$; both sets of values converge quickly to a limit which we estimate, using quadratic extrapolation (versus $1/L^2$), as $p_c = 0.8900(2)$.

The finite-size scaling relations for ρ_p, τ, and m, cited above, are satisfied to good precision for $p = 0.8900$; the data for the order parameter are shown in the inset of Fig. 2. Including results for $L = 640$, however, we find small but significant curvatures in the graphs of $\ln \rho_p$ and $\ln \tau$ versus $\ln L$, indicating that p_c is slightly larger than 0.8900. (The curvatures are:

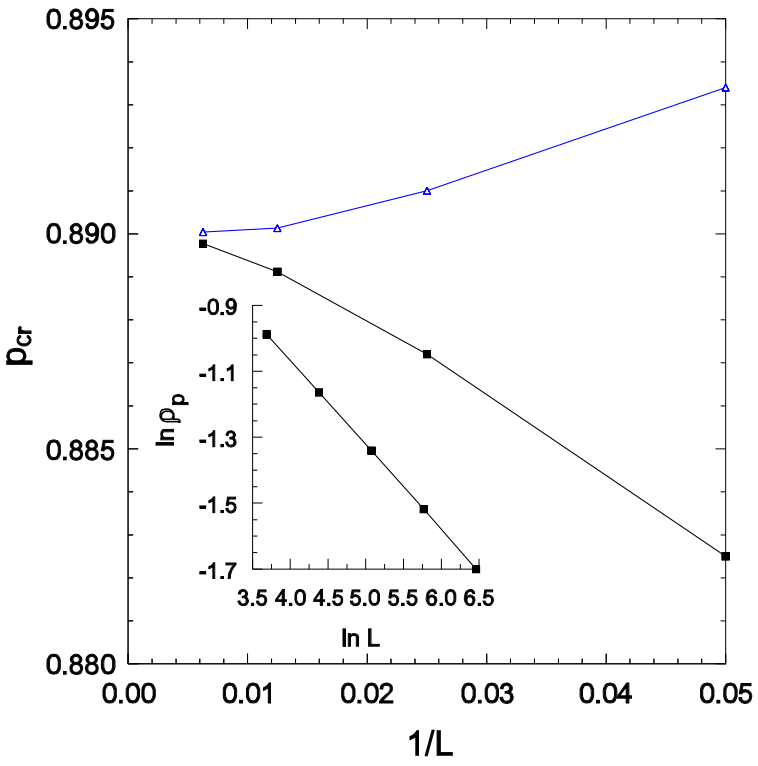

FIG. 2: (Color online) Values $p_\times$ and p_q associated, respectively, with moment ratio crossings (lower) and minima in the reduced fourth cumulant (upper), versus $1/L$, for $D = 0.5$. Inset: Order parameter ρ_p versus system size, for $D = 0.5$ and $p = 0.89$.

-0.0019(4) in the case of ρ_p and -0.009(3) for τ.) We perform additional simulations for $L = 640$ at $p = 0.8903$ and 0.8906, and then calculate the curvatures of the graphs of $\ln \rho_p$ and $\ln \tau$ versus $\ln L$ for diverse values of p in the interval [0.89, 0.8903], using polynomial interpolation of the simulation data as necessary, to estimate the quantities of interest at intermediate points. We observe no significant curvature for p in the interval [0.89004, 0.89010], leading to our final estimate, $p_c = 0.89007(3)$, for $D = 0.5$. The associated critical parameters are $\beta/\nu_\perp = 0.252(2)$, $z = 1.573(10)$, and $m = 1.1758(24)$. (Note that the principal source of uncertainty in these estimates is the uncertainty in p_c itself.)

The data for the particle density ρ_{part} scales in the same manner as the pair density: at the critical point, we find, to good precision, $\rho_{part} \simeq \rho_{part,c} + AL^{-\beta/\nu_\perp}$, using the same value for $\beta/\nu_\perp$ as found in the analysis of the pair density. (For $D = 0.5$, for example, the limiting particle density is $\rho_{part,c} = 0.2321(2)$.) The moment ratio associated with the particle density, $m_{part} \equiv \langle(\rho_{part} - \rho_{part,c})^2\rangle / \langle\rho_{part} - \rho_{part,c}\rangle^2$, behaves similarly to the moment ratio associated with pairs; for $D = 0.5$ we find $m_{part,c} = 1.177(5)$.

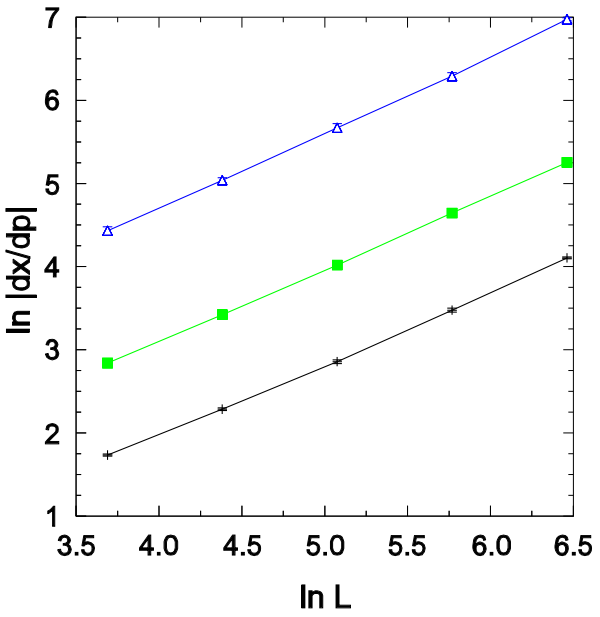

FIG. 3: (Color online) Derivatives $|dm/dp|$ (lower), $d\ln\tau/dp$ (upper), and $d\ln\rho_p/dp$ (middle) versus L for $D = 0.5$.

The simulation data also permit a direct estimate of the exponent $\nu_\perp$, albeit with somewhat limited precision. Finite-size scaling implies that the derivatives $|dm/dp|$, $d\ln\tau/dp$ and $d\ln\rho_p/dp$, evaluated at the critical point, follow $|dx/dp| \propto L^{1/\nu_\perp}$ (here x stands for any of the quantities mentioned). We estimate the derivatives via least-squares linear fits to the data on an interval that includes p_c. (The intervals are small enough that the graphs show no significant curvature.) Power-law dependence of the derivatives on system size is verified in Fig. 3. Linear fits to the data for the three largest sizes, for m, $\ln\rho_p$, and $\ln\tau$ yield $1/\nu_\perp = 0.900(4)$, $0.940(26)$ e $0.891(7)$, respectively, leading to the estimate $\nu_\perp = 1.10(2)$. The simulations and analyses described above were repeated for diffusion rates $D = 0.1$ and 0.9, yielding the results shown in Table I. For $D = 0.9$, finite-size corrections are much stronger than for the smaller diffusion rates, and we found it necessary to extend the study to larger system sizes to obtain reliable results. The values listed in Table I are based on studies using $L = 320$, 640, 1280, and 2560, in this case.

D	p_c	β/ν	z	$\nu_\perp$	m_p
0.1	0.91720(1)	0.252(1)	1.584(11)	1.11(4)	1.173(1)
0.5	0.89007(3)	0.252(2)	1.573(10)	1.10(2)	1.1758(2)
0.9	0.83470(5)	0.253(1)	1.573(5)	1.12(3)	1.178(2)
DP		0.25208(5)	1.5807(1)	1.096854(4)	1.1736(1)

TABLE I: Critical exponent values for the PCPDP and DP; figures in parentheses denote uncertainties. DP values from Refs. [16] and [17].

IV. CONCLUSIONS

We study a version of the pair contact process in which nearest-neighbor particle pairs (but not isolated particles) diffuse. The results of quasistationary simulations, for $\beta/\nu_\perp$, z, $\nu_\perp$, and the moment ratio m, confirm to good precision that the scaling properties of this model coincide with those of directed percolation. This conclusion is what one would expect on the basis of universality: diffusion of pairs changes nothing fundamental in the propagation of activity or in the space of absorbing configurations of the original pair contact process. The situation is quite different from that of the PCP with diffusion of *particles*: the critical behavior of the PCPD is still not fully understood, and is evidently subject to much stronger corrections to scaling than is the model studied here (PCPDP). Thus our conclusion that the PCPDP belongs to the directed percolation universality class does not imply that the same holds (or does not hold) for the PCPD.

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